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A numerical strategy for coarse-graining two-dimensional atomistic models at finite temperature: the membrane case

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Abstract

We present a numerical strategy to compute ensemble averages of coarse-grained two-dimensional membrane-like models. The approach consists in generalizing to these two-dimensional models a one-dimensional strategy exposed in [Blanc, Le Bris, Legoll, Patz, JNLS 2010, [6]], which is based on applying the ergodic theorem to Markov chains. This may be considered as a first step towards computing the constitutive law associated to such models, in the thermodynamic limit.

1 Introduction

A standard problem in materials science is the computation of canonical averages. As an example, consider a system of P particles, at positions $u = (u^1, \ldots, u^P) \in \mathbb{R}^{3P}$, and assume that its energy is given by a two-body interaction:

$$E(u) = \frac{1}{2} \sum_{i \neq j} W(u^i - u^j). \tag{1.1}$$

Given an observable $A : \mathbb{R}^{3P} \to \mathbb{R}$, and $\beta > 0$ the inverse of the temperature, the canonical ensemble average of A is defined by (see e.g. [11])

$$\langle A \rangle = \frac{\displaystyle\int_{\Omega^P} A(u) e^{-\beta E(u)} du}{\displaystyle\int_{\Omega^P} e^{-\beta E(u)} du}, \tag{1.2}$$

where $\Omega \subset \mathbb{R}^3$ is the macroscopic domain in which the particles are assumed to lie.

Such canonical averages relate the macroscopic properties of a system to the elementary phenomena at the microscopic scale, which are modelled by the atomistic energy (1.1). For instance, the bulk pressure in a fluid is given by (1.2), for the observable

$$A(u) = \rho T - \frac{1}{3|\Omega|} \sum_{i=1}^{P} u^i \cdot \frac{\partial E}{\partial u^i}(u),$$

where T is the temperature and ρ the density. If the atoms are non-interacting, then $E \equiv 0$ and we recover Mariotte's law for ideal gas. In general, the relation (1.2) (with the above choice for A) allows to compute the pressure of a liquid at a given density and temperature, and hence to obtain its macroscopic constitutive law, based on the microscopic model (1.1).

The integrals in (1.2) involve $3P$ variables, and this number is extremely large when one considers a macroscopic sample of matter. Therefore, a direct computation of $\langle A \rangle$, by standard quadrature rules (using Gauss integration points), is not tractable. Several approaches have been proposed to deal with such problems (see e.g. [9] for a theoretical and numerical comparison of those). The approach we will follow here is to use the so-called overdamped Langevin dynamics. This stochastic dynamics reads

$$du = -\nabla E(u)dt + \sqrt{2/\beta}\, dB_t, \tag{1.3}$$

where B_t is a Brownian motion in dimension $3P$. This dynamics is hence a steepest descent (according to the forces $-\nabla E(u)$), modified by a random noise, the magnitude of which is scaled by the temperature: the larger the temperature, the stronger the noise. The dynamics (1.3) is interesting because of the following ergodicity result: under general assumptions on the energy E, we have

$$\langle A \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T A(u(t))dt \tag{1.4}$$

for (almost) all initial conditions $u(0)$. In the long time limit, the random number $\dfrac{1}{T}\displaystyle\int_0^T A(u(t))dt$ converges to a deterministic number, which is the canonical average of interest.

Thus, in order to compute (1.2), a standard approach consists in simulating the evolution of the system according to (1.3) (this can be done even for large systems), and averaging the quantity $A(u(t))$ along the obtained trajectory. The equation (1.4) ensures that the time average of $A(u(t))$ converges to the desired quantity $\langle A \rangle$ in the long time limit. In practice, the equation (1.3) is numerically integrated with the forward Euler scheme

$$u_{m+1} = u_m - \Delta t\, \nabla_u E(u_m) + \sqrt{2\Delta t \beta^{-1}}\, G_m$$

with the time step Δt, where G_m is a vector of Gaussian random variables in dimension $3P$ (all components of G_m are independent from each other, and they

are all distributed according to a Gaussian law of mean 0 and variance 1). In turn, following (1.4), the canonical average (1.2) is approximated by

$$\langle A \rangle \approx \lim_{M \to \infty} \frac{1}{M} \sum_{m=1}^{M} A\left(u_m\right).$$

We described above how to compute the canonical average (1.2) using the overdamped Langevin dynamics (1.3). We point out that we give *no physical meaning* to this dynamics, which is only considered here as a *numerical tool* to sample the Gibbs measure and allow efficient computation of canonical averages.

As pointed out above, several such numerical tools have been proposed in the literature, and among them, the Langevin equation, which is closer to physical, Hamiltonian dynamics than the overdamped Langevin dynamics (1.3). The Langevin dynamics reads

$$\begin{aligned} du &= M^{-1} p \, dt, \\ dp &= -\nabla E(u) dt - \gamma M^{-1} p \, dt + \sqrt{2\gamma/\beta} \, dB_t, \end{aligned} \tag{1.5}$$

where $u \in \mathbb{R}^{3P}$ represents the position of the atoms, $p \in \mathbb{R}^{3P}$ their momentum, M is a mass matrix, and $\gamma > 0$ is a parameter. This dynamics shares the same ergodicity property as the overdamped Langevin dynamics: for any $\gamma > 0$, the convergence (1.4) holds along trajectories of (1.5).

Note that, when $\gamma = 0$, we recover from (1.5) the standard Hamiltonian dynamics (Newtonian dynamics). When $\gamma > 0$, the Langevin dynamics includes some friction and some random noise, which is, as for the overdamped Langevin dynamics, scaled by the temperature. Finally, in the limit $\gamma \to \infty$, and up to some time rescaling, the Langevin dynamics (1.5) converges to the overdamped Langevin dynamics (1.3) (see e.g. [24, Sec. 2.2.4]).

In many cases, the observable A of interest does not depend on all positions u^i, but only on a few of them. Our aim here is to derive simpler methods for computing canonical averages in such a case, based on a coarse-graining strategy. Such methods were used in [6] for one-dimensional models (see also [23]), and we adapt here the strategy to a two-dimensional membrane-like model.

One possible approach to address such question is the *QuasiContinuum Method* (QCM). It was first introduced in [36, 37], and further developed in [21, 28, 29, 33, 34, 38], in the zero temperature case. It has been theoretically studied in [1, 2, 3, 4, 5, 7, 13, 16, 17, 18, 26, 27, 31]. See also [8, 22] for some review articles. The method was adapted to the finite temperature case in [15], resulting in a coarse-graining strategy to compute ensemble averages. Similar strategies were also proposed in [10, 25].

In essence, any coarse-graining approach aims at using the fact that A depends only on the positions of some representative atoms at positions $u_r \in \Omega^{P_r}$, with $P_r \ll P$. This is usually done by writing formally

$$\langle A \rangle = \frac{1}{Z_P} \int_{\Omega^P} A(u_r) e^{-\beta E(u)} du = \frac{1}{Z_{P_r}} \int_{\Omega^{P_r}} A(u_r) e^{-\beta E_{CG}(u_r)} du_r,$$

where

$$Z_P = \int_{\Omega^P} \exp\left(-\beta E(u)\right) du, \quad Z_{P_r} = \int_{\Omega^{P_r}} \exp\left(-\beta E_{CG}(u_r)\right) du_r,$$

and where

$$E_{CG}(u_r) = -\frac{1}{\beta} \ln \left[\int_{\Omega^{P-P_r}} \exp\left(-\beta E(u)\right) d\hat{u}_r \right] \tag{1.6}$$

is the coarse-grained energy. In (1.6), the notation $d\hat{u}_r$ indicates that we integrate over all variables except u_r. The question then reduces to computing the coarse-grained energy E_{CG}, which can be considered as the free energy of the system, for the collective variable (or reaction coordinate) u_r.

Note that $E_{CG}(u_r)$ depends on P, and is in general difficult to compute for a given value of P_r and P. However, one may hope that its expression simplifies in the limit when

$$P_r \text{ is fixed, } P \to \infty.$$

This is the case for instance in dimension one, in the case of nearest-neighbour interactions, as it is recalled in Section 1.1 below.

Rather than fixing β and letting $P \to \infty$, as described above, another asymptotic regime is to keep P and P_r fixed and let β go to $+\infty$ (vanishing temperature). This is the regime considered by the QCM approach, which is based, roughly speaking, on using a harmonic approximation of $E(u)$ in (1.6). This then allows to compute explicitly $E_{CG}(u_r)$.

The sequel of this article is organized as follows. In Section 1.1, we consider one-dimensional chains of atoms, and recall our results of [6]. We next present in Section 1.2 the two-dimensional membrane-like models we consider here, and the questions we are after. Section 2 is dedicated to the derivation of our numerical strategy, which is very much inspired by our previous works on one-dimensional models. The outcome of this derivation is an algorithm, that we have summarized in Section 2.3. Numerical results obtained with this algorithm are presented (and compared with the reference model results) in Section 3.

1.1 Dimension one

In [6], we proposed a methodology to deal with one-dimensional models. Although the method allows to handle models with any finite range interaction, we recall it here in the special case of nearest-neighbour and next-to-nearest-neighbour interaction, refering to [6, 23] for more details.

Consider a chain of P atoms at positions $u^i \in \mathbb{R}$, with an energy of nearest-neighbour type:

$$E(u) = \sum_{i=0}^{P-1} W\left(\frac{u^{i+1} - u^i}{h}\right), \tag{1.7}$$

where $h = 1/P$ is the average spacing of the atoms, and is assumed here to be equal to the characteristic length of the potential (as the equilibrium length of

$z \mapsto W(z)$ is assumed to be of order 1, the equilibrium length of $z \mapsto W(z/h)$ is of the order of h). To remove the translation invariance of the energy, we set $u^0 = 0$.

As explained above, we consider the canonical average of observables depending only on a few atoms of the system. To simplify the setting, we assume that A depends only on u^P. Thus, the quantity we wish to compute is

$$\langle A \rangle_P = \frac{1}{Z_P} \int_{\mathbb{R}^P} A\left(u^P\right) \exp\left[-\beta \sum_{i=0}^{P-1} W\left(\frac{u^{i+1}-u^i}{h}\right)\right] du,$$

where $Z_P = \displaystyle\int_{\mathbb{R}^P} \exp\left[-\beta \sum_{i=0}^{P-1} W\left(\frac{u^{i+1}-u^i}{h}\right)\right] du$. More precisely, we are going to compute the limit of $\langle A \rangle_P$ when $P \to \infty$, that is in the thermodynamic limit, when the number of atoms present in the system diverges.

Changing variables according to

$$y_i := \frac{u^i - u^{i-1}}{h}, \quad i = 1, \ldots, P, \tag{1.8}$$

which implies $u^P = \dfrac{1}{P} \displaystyle\sum_{i=1}^{P} y_i$, we have

$$\langle A \rangle_P = \frac{1}{Z_P} \int_{\mathbb{R}^P} A\left(\frac{1}{P}\sum_{i=1}^{P} y_i\right) \exp\left[-\beta \sum_{i=1}^{P} W(y_i)\right] dy, \tag{1.9}$$

with

$$Z_P = \int_{\mathbb{R}^P} \exp\left[-\beta \sum_{i=1}^{P} W(y_i)\right] dy.$$

Thus, (1.9) may be interpreted as the expectation value of a sequence of independent identically distributed (i.i.d.) variables:

$$\langle A \rangle_P = \mathbb{E}\left[A\left(\frac{1}{P}\sum_{i=1}^{P} Y_i\right)\right],$$

where Y_i is a sequence of i.i.d. variables distributed according to the law $d\mu(y) = Z^{-1}\exp(-\beta W(y))dy$, and $Z = \int_{\mathbb{R}} \exp(-\beta W(y))dy$. For finite (and large) P, the quantity $\langle A \rangle_P$ is not particularly easy to compute. However, its limit when $P \to \infty$ is easy to compute. Indeed, applying the law of large numbers [35], we know that $\dfrac{1}{P}\displaystyle\sum_{i=1}^{P} Y_i$ converges to the mean $\mathbb{E}(Y_i)$ of the random variables Y_i, and we hence have (see [6]):

$$\lim_{P\to\infty} \langle A \rangle_P = A(y^\star), \quad y^\star := \mathbb{E}(Y_i) = \frac{\displaystyle\int_{\mathbb{R}} y \exp(-\beta W(y))dy}{\displaystyle\int_{\mathbb{R}} \exp(-\beta W(y))dy}. \tag{1.10}$$

Remark 1 *Choosing $A(y) = y$ in the above relation, we observe that $y^\star$ satisfies $y^\star = \lim_{P\to\infty} \langle u^P \rangle_P$. In the specific one-dimensional nearest-neighbour case discussed here, we actually have $y^\star = \langle u^P \rangle_P$ for any P. Likewise, for any P and any $1 \le i \le P$, we have $y^\star = \langle y_i \rangle_P = \langle \dfrac{u^i - u^{i-1}}{h} \rangle_P$.*

The property (1.10) holds under mild assumptions on A and W. The only important constraint is that $\exp(-\beta W)$ should be integrable over the real line. Actually, finer results may be easily obtained, as for instance Theorem 1 of [6].

In the case of next-to-nearest-neighbour interaction, it is possible to apply the same kind of strategy, but it is much more involved. Assume now that, instead of (1.7), the energy reads

$$E(u) = \sum_{i=0}^{P-1} W_1\left(\frac{u^{i+1} - u^i}{h}\right) + \sum_{i=1}^{P-1} W_2\left(\frac{u^{i+1} - u^{i-1}}{h}\right). \tag{1.11}$$

Again, we assume that the observable A depends only on the right-end atom position u^P, and that $u^0 = 0$. Then, using the same change of variables (1.8), we have

$$\begin{aligned} \langle A \rangle_P &= \frac{1}{Z_P} \int_{\mathbb{R}^P} A\left(u^P\right) \exp\left[-\beta E(u)\right] du \\ &= \frac{1}{Z_P} \int_{\mathbb{R}^P} A\left(\frac{1}{P}\sum_{i=1}^{P} y_i\right) \exp\left[-\beta \sum_{i=1}^{P} W_1(y_i)\right] \\ &\qquad \times \exp\left[-\beta \sum_{i=1}^{P-1} W_2(y_i + y_{i+1})\right] dy. \end{aligned} \tag{1.12}$$

Here, instead of i.i.d. variables, we may identify a Markov chain structure. Introduce indeed

$$k(a,b) = \exp\left[-\frac{\beta}{2} W_1(a) - \frac{\beta}{2} W_1(b) - \beta W_2(a+b)\right].$$

Then we can recast (1.12) as

$$\begin{aligned} \langle A \rangle_P = \frac{1}{Z_P} \int_{\mathbb{R}^P} A\left(\frac{1}{P}\sum_{i=1}^{P} y_i\right) \exp\left[-\frac{\beta}{2} W_1(y_1) - \frac{\beta}{2} W_1(y_P)\right] \\ \times \prod_{i=1}^{P-1} k(y_i, y_{i+1}) dy. \end{aligned} \tag{1.13}$$

For the sake of simplicity, assume now that $\displaystyle\int_{\mathbb{R}} k(a,b)\, db = 1$. Then we can introduce a Markov chain $\{Y_i\}_{i\ge 0}$ of kernel k, namely such that $k(a,b) = \mathbb{P}(Y_{i+1} =$

$b \mid Y_i = a$), and recast (1.13) as

$$\langle A \rangle_P = \frac{\mathbb{E}\left[A\left(\frac{1}{P}\sum_{i=1}^P Y_i\right)\exp\left(-\frac{\beta}{2}W_1(Y_1) - \frac{\beta}{2}W_1(Y_P)\right)\right]}{\mathbb{E}\left[\exp\left(-\frac{\beta}{2}W_1(Y_1) - \frac{\beta}{2}W_1(Y_P)\right)\right]}.$$

Applying next the law of large numbers (this time for Markov chains, rather than for i.i.d. variables as previously), we can identify $\lim_{P\to\infty}\langle A\rangle_P$.

In general, the quantity $\int_{\mathbb{R}} k(a,b)\,db$ depends on a, and is not equal to 1. So the above discussion needs to be amended. It turns out that it is nevertheless possible to identify a Markov chain structure in (1.12). Hence, applying asymptotic theorems (namely law of large numbers type results) for this setting (see e.g. [35]), we have (see [6] for the details):

$$\lim_{P\to\infty}\langle A\rangle_P = A(y^\star), \quad y^\star = \int_{\mathbb{R}} y\left(\psi_1(y)\right)^2 dy, \tag{1.14}$$

where ψ_1^2 is the invariant measure of the transition kernel of the Markov chain, that is, the solution of

$$\mathcal{P}\psi_1 = \lambda\psi_1, \quad \lambda = \max \mathrm{Spectrum}(\mathcal{P}), \tag{1.15}$$

where the transition operator $\mathcal{P}$ is defined on functions $\phi : \mathbb{R} \to \mathbb{R}$ by

$$\left(\mathcal{P}\phi\right)(x) = \int_{\mathbb{R}} \phi(y)\exp\left[-\frac{\beta}{2}W_1(x) - \frac{\beta}{2}W_1(y) - \beta W_2(x+y)\right] dy.$$

Note that, using standard tools of spectral theory, it is possible to prove that, under some reasonable assumptions, problem (1.15) has a unique solution (we refer to [6] for the details).

Remark 2 *As in the nearest-neighbour case, choosing $A(y) = y$ in (1.14), we have $y^\star = \lim_{P\to\infty}\langle u^P\rangle_P$. Note that we also have*

$$y^\star = \lim_{P\to\infty}\langle y_i\rangle_P = \lim_{P\to\infty}\langle\frac{u^i - u^{i-1}}{h}\rangle_P$$

for any $1 \ll i \ll P$. Otherwise stated, $y^\star$ is the average (rescaled) elongation of any bond which is in the bulk of the chain.

Before moving on to the two-dimensional setting, let us briefly describe one application of the above strategy. We have considered until now chains of atoms at rest, that is, submitted to *no external force*. The energy of the system reads (1.7) (or (1.11)). Choosing $A(u) = u$ in (1.10) (or (1.14)), we see that $y^\star$ is the average elongation of the system, at a given finite temperature (macroscopic equilibrium length). It turns out that the above strategy can be easily extended to treat the case when some external force is applied to the right-end atom of

the chain (at position u^P), while we again impose the position of the left-end atom: $u^0 = 0$. In this case, the energy, rather than (1.7), reads

$$E_f(u) = \sum_{i=0}^{P-1} W\left(\frac{u^{i+1} - u^i}{h}\right) - f\frac{u^P}{h},$$

and the average length of the chain, at the inverse temperature β, and when a force f is applied at the right-end, reads

$$\langle A\rangle_P^f = \frac{1}{Z_P}\int_{\mathbb{R}^P} A\left(u^P\right)\exp\left[-\beta E_f(u)\right]du,$$

for $A(u) = u$. Following the same arguments as above (see [23] for details), we can compute $y_f^\star = \lim_{P\to\infty}\langle u^P\rangle_P^f$, which is the average *elongation* of the system when submitted to the external *force* f. We thus have computed the constitutive law of the chain (namely the relationship between force and elongation), at finite temperature.

1.2 Setting of the problem

We now turn to describing the problem we address in this article. The above treatment of the one-dimensional setting will be used as a bottom-line to treat the case at hand here, namely two-dimensional membrane-like models. In contrast to the one-dimensional case, we are not able to prove the convergences we claim. However, we believe that the one-dimensional proofs are sufficient to allow for the approximations we are going to make. Extensive numerical results reported in Section 3 below show the accuracy of our approximations.

We consider a two-dimensional atomistic system, where each atom has a *scalar* degree of freedom. The mechanical interpretation is that the system is a *membrane*, and the degree of freedom is the height of the atom (see Figure 1).

We hence consider a two-dimensional set of $P = (N+1)^2$ atoms at positions

$$u^{i,j} \in \mathbb{R}, \quad 0 \le i,j \le N.$$

We assume a nearest-neighbour interaction, and thus write the energy as

$$E\left(\left\{u^{i,j}\right\}\right) = \sum_{0\le i,j\le N} \sum_{\substack{0\le k,l\le N \\ i\le k\le i+1,\ j\le l\le j+1 \\ (k-i)+(l-j)=1}} W\left(\frac{u^{k,l} - u^{i,j}}{h}\right). \tag{1.16}$$

Note that, as in (1.7), we have rescaled the relative position by the factor $h = 1/N$. Likewise, we consider in the above sum oriented bonds, from left to right or bottom to top (but not the contrary). Finally, as in the one-dimensional case, we do not have to assume W to be an even function. The energy (1.16) is translation

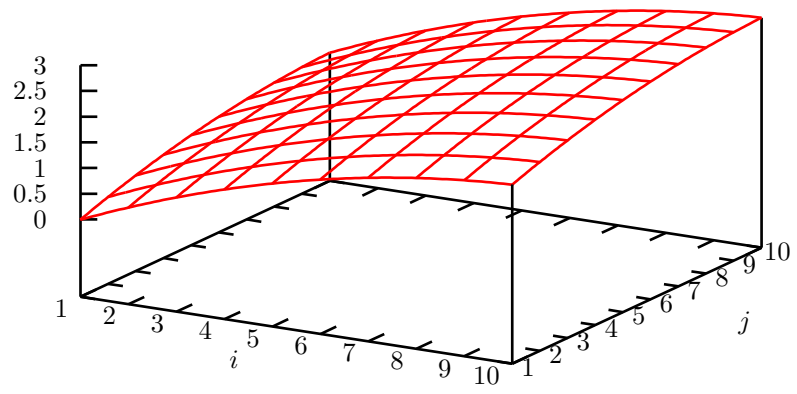

Figure 1: Schematic representation of the system: atoms are set on a two-dimensional lattice, and have a unique degree of freedom, which is their height.

invariant, so we fix in the sequel $u^{0,0} = 0$ to remove this invariance. Our aim is to compute the canonical average of an observable A that only depends on $u^{N,N}$, with respect to the Gibbs measure associated to the energy (1.16). This quantity reads

$$\langle A \rangle_N = Z_N^{-1} \int_{\mathbb{R}^{(N+1)^2-1}} A\left(u^{N,N}\right) \, \overline{\mu}_N\left(\left\{u^{i,j}\right\}\right) \prod_{0 \le i,j \le N, \ (i,j) \neq (0,0)} du^{i,j}, \quad (1.17)$$

where

$$\overline{\mu}_N\left(\left\{u^{i,j}\right\}\right) = \exp(-\beta E\left(\left\{u^{i,j}\right\}\right)) \quad (1.18)$$

is the non-normalized Gibbs measure, and

$$Z_N = \int_{\mathbb{R}^{(N+1)^2-1}} \overline{\mu}_N\left(\left\{u^{i,j}\right\}\right) \prod_{0 \le i,j \le N, \ (i,j) \neq (0,0)} du^{i,j}$$

is the normalization constant. Our exact aim is to compute $\langle A \rangle_N$ in the *thermodynamics limit*, namely $\lim_{N \to \infty} \langle A \rangle_N$.

As in [6], we aim at describing a numerical strategy to compute $\lim_{N \to \infty} \langle A \rangle_N$ that builds on the specificity that the observable A under study depends *only* on $u^{N,N}$, and not on *all* the atom positions $\left\{u^{i,j}\right\}_{0 \le i,j \le N}$. As we will see below, we are also able to handle observables that depend only of $u^{0,N}$ or $u^{N,0}$, and, more generally, of $u^{0,N}$, $u^{N,0}$ and $u^{N,N}$. We build this strategy in Section 2, and

obtain the algorithm summarized in Section 2.3. Numerical results are reported in Section 3.

Remark 3 *In dimension one, in addition to computing* $\lim_{P\to\infty} \langle A \rangle_P$ *(as recalled in Section 1.1), it is also possible, using a large deviation principle strategy, to compute the coarse-grained energy* E_{CG} *defined by* (1.6)*. We refer to [6, 23] for the details. In dimension two, such a problem is known to be very difficult, and very few theoretical results are known. See for instance [19, 12, 20, 30]. This is why we concentrate here on the simpler question of computing the average of an observable.*

2 Numerical strategy

This section is dedicated to the construction of our numerical strategy. It is quite involved from the technical viewpoint. For the sake of clarity, we have summarized in Section 2.3 below the resulting algorithm which has eventually to be implemented.

We first rewrite the energy (1.16) using the increments between the atoms. Introducing

$$\begin{aligned} x_{i,j} &= \frac{u^{i,j} - u^{i-1,j}}{h}, \quad 1 \le i \le N, \quad 0 \le j \le N, \\ y_{i,j} &= \frac{u^{i,j} - u^{i,j-1}}{h}, \quad 0 \le i \le N, \quad 1 \le j \le N, \end{aligned}$$

we have

$$E\left(\left\{u^{i,j}\right\}\right) = \sum_{1\le i,j\le N} W(x_{i,j}) + W(y_{i,j}) + \sum_{i=1}^{N} W(x_{i,0}) + \sum_{j=1}^{N} W(y_{0,j}). \quad (2.1)$$

This change of variables is not one-to-one: $(N+1)^2 - 1$ variables are involved in (1.16), whereas $2N^2 + 2N$ variables are involved in (2.1). The difference is accounted for by imposing the geometric constraints

$$x_{i,j} + y_{i-1,j} = y_{i,j} + x_{i,j-1},$$

for $1 \le i, j \le N$.

In the variables $(x_{i,j}, y_{i,j})$, the non-normalized Gibbs measure $\overline{\mu}_N$ reads

$$\prod_{1\le i,j\le N} f(x_{i,j})\, f(y_{i,j})\; \delta_0\left(x_{i,j} + y_{i-1,j} - y_{i,j} - x_{i,j-1}\right) \times \prod_{1\le i\le N} f(x_{i,0}) \prod_{1\le j\le N} f(y_{0,j}), \quad (2.2)$$

with

$$f(x) = \exp(-\beta W(x)),$$

and we recast (1.17) as

$$\langle A\rangle_N = Z_N^{-1}\int A\left(\frac{1}{N}\sum_{i=1}^{N}(x_{i,i}+y_{i,i})\right)\prod_{1\le i\le N} f(x_{i,0})\prod_{1\le j\le N} f(y_{0,j}) \\ \times\prod_{1\le i,j\le N} f(x_{i,j})\,f(y_{i,j})\;\delta_0\left(x_{i,j}+y_{i-1,j}-y_{i,j}-x_{i,j-1}\right). \quad (2.3)$$

Based on our one-dimensional study (recalled in Section 1.1), our first assumption is

$$\textbf{[H1]}\quad \text{the boundary terms of the Gibbs measure (second line of (2.2)) are disregarded.} \quad (2.4)$$

Thus, we approximate (2.3) by

$$\langle A\rangle_N \approx \langle A\rangle_N^{\mathrm{NoBoundr}}, \quad (2.5)$$

where

$$\langle A\rangle_N^{\mathrm{NoBoundr}} = Z_N^{-1}\int A\left(\frac{1}{N}\sum_{i=1}^{N}(x_{i,i}+y_{i,i})\right)\mu_N\left(\{x_{i,j}\},\{y_{i,j}\}\right),$$

with

$$\mu_N\left(\{x_{i,j}\},\{y_{i,j}\}\right) = \prod_{1\le i,j\le N} f(x_{i,j})f(y_{i,j})\delta_0\left(x_{i,j}+y_{i-1,j}-y_{i,j}-x_{i,j-1}\right).$$

Again based on the one-dimensional study, we assume that we can apply (1.14) and Remark 2, so that

$$\textbf{[H2]}\quad \lim_{N\to+\infty}\langle A\rangle_N^{\mathrm{NoBoundr}} = A(x^\star+y^\star), \quad (2.6)$$

where

$$x^\star = \lim_{N\to+\infty} Z_N^{-1}\int x_{k,l}\;\mu_N\left(\{x_{i,j}\},\{y_{i,j}\}\right), \quad (2.7)$$

$$y^\star = \lim_{N\to+\infty} Z_N^{-1}\int y_{k,l}\;\mu_N\left(\{x_{i,j}\},\{y_{i,j}\}\right), \quad (2.8)$$

where k and l are any integers such that $1\ll k,l\ll N$. We implicitly assume in (2.7)-(2.8) that $x^\star$ and $y^\star$ do not depend on k,l, provided $1\ll k,l\ll N$. Collecting (2.5) and (2.6), we thus write

$$\lim_{N\to+\infty}\langle A\rangle_N \approx A(x^\star+y^\star). \quad (2.9)$$

All the sequel of this section is dedicated to the computation of (an approximation of) $x^\star$ and $y^\star$.

Remark 4 *Based on the knowledge of $x^\star$ and $y^\star$, we can compute $A(x^\star + y^\star)$, which is assumed to be an approximation of the average of $A(u^{N,N})$, according to (2.9). Using the same assumptions, our strategy leads us to approximate the average of $A(u^{N,0})$ and $A(u^{0,N})$ by $A(x^\star)$ and $A(y^\star)$, respectively. We will show in Section 3 that $A(x^\star + y^\star)$, $A(x^\star)$ and $A(y^\star)$ are indeed good approximations of the average of $A(u^{N,N})$, $A(u^{N,0})$ and $A(u^{0,N})$, respectively.*

As pointed out above, our strategy can straighforwardly be extended to the case when the observable A depends on $u^{N,N}$, $u^{N,0}$ and $u^{0,N}$, although we have not numerically tested such cases in the sequel.

2.1 Numerical computation of $x^\star$ and $y^\star$

Our strategy consists in setting an appropriate Markov chain structure, as we did for the one-dimensional next-to-nearest-neighbour interaction case (see Section 1.1). The variables $x_{i,j}$ in (2.7) are indexed by (i,j), which belongs to a subset of $\mathbb{Z}^2$, on which there is no natural ordering. Rather than considering the variables $x_{i,j}$, we are going to consider the row of variables $\{x_{i,j}\}_{1\leq i\leq N}$, indexed by j. The advantage is that there is a natural ordering between these rows of variables.

We now proceed in details. For any $1 \leq j \leq N$, define

$$x_{:,j} = (x_{1,j}, \ldots, x_{N,j}) \in \mathbb{R}^N, \quad y_{:,j} = (y_{1,j}, \ldots, y_{N,j}) \in \mathbb{R}^N.$$

We thus have

$$\mu_N \quad = \quad \prod_{j=1}^{N} F(x_{:,j})\, F(y_{:,j})\; \delta_0(x_{:,j} + \tau y_{:,j} - y_{:,j} - x_{:,j-1}), \qquad (2.10)$$

where τ is the Bernoulli shift, i.e. $(\tau y)_i = y_{i-1}$, and F is the direct product

$$F(x_{:,j}) = \prod_{i=1}^{N} f(x_{i,j}), \quad F(y_{:,j}) = \prod_{i=1}^{N} f(y_{i,j}).$$

With this notation, (2.7) reads

$$x^\star = \lim_{N\to+\infty} Z_N^{-1} \int x_{k,l} \; \prod_{j=1}^{N} F(x_{:,j})\, F(y_{:,j})\; \delta_0(x_{:,j} + \tau y_{:,j} - y_{:,j} - x_{:,j-1}). \quad (2.11)$$

We now follow a strategy based on the so-called transfer operators (or transfer matrices; see for instance [35, Chapter I, Section 12]). Let us define the transfer operator $\mathcal{P}$ by

$$\begin{aligned}(\mathcal{P}\varphi)(x,y) \quad &= \quad F(x)F(y) \int_{\mathbb{R}^N\times\mathbb{R}^N} \varphi(t,z)\; \delta_0(t + \tau z - z - x)\; dz\; dt \\ &= \quad F(x)F(y) \int_{\mathbb{R}^N} \varphi(x + z - \tau z, z)\; dz\end{aligned}$$

for any function φ defined on $\mathbb{R}^N \times \mathbb{R}^N$. The adjoint operator reads

$$(\mathcal{P}^\star\varphi)(x,y) = F(x+\tau y - y)\int_{\mathbb{R}^N} F(z)\ \varphi(x+\tau y - y, z)\ dz.$$

We can compute the law of $(x_{:,l}, y_{:,l})$ by integrating (2.10) over all variables except $(x_{:,l}, y_{:,l})$. The interest of introducing $\mathcal{P}$ and $\mathcal{P}^\star$ is that we can now recast (2.11) in the simple form

$$x^\star = \lim_{N\to+\infty} \frac{\displaystyle\int_{\mathbb{R}^N\times\mathbb{R}^N} x_{k,l}\ \mu_l(x_{:,l}, y_{:,l})\ dx_{:,l}\ dy_{:,l}}{\displaystyle\int_{\mathbb{R}^N\times\mathbb{R}^N} \mu_l(x_{:,l}, y_{:,l})\ dx_{:,l}\ dy_{:,l}} \tag{2.12}$$

with

$$\mu_l(x_{:,l}, y_{:,l}) = \left(\mathcal{P}^{N-l}\varphi_0\right)(x_{:,l}, y_{:,l})\ \left((\mathcal{P}^\star)^{l-1}\varphi_1\right)(x_{:,l}, y_{:,l}), \tag{2.13}$$

where $\varphi_0(x_{:,N}, y_{:,N}) = F(x_{:,N})\,F(y_{:,N})$ and $\varphi_1 = 1$. Assuming N large and $1 \ll l \ll N$, the iterations of $\mathcal{P}$ and $\mathcal{P}^\star$ converge, up to renormalization, to the spectral projection on the highest eigenvector of $\mathcal{P}$ and $\mathcal{P}^\star$, respectively. Hence, the law of $(x_{:,l}, y_{:,l})$ is

$$\mu_l(x_{:,l}, y_{:,l}) = \frac{\mu(x_{:,l}, y_{:,l})\ \mu^\star(x_{:,l}, y_{:,l})}{\int_{\mathbb{R}^N\times\mathbb{R}^N} \mu(x_{:,l}, y_{:,l})\ \mu^\star(x_{:,l}, y_{:,l})\ dx_{:,l}\ dy_{:,l}} \tag{2.14}$$

where μ and $\mu^\star$ are functions defined on $\mathbb{R}^N \times \mathbb{R}^N$ satisfying

$$\left\{\begin{array}{l} \mathcal{P}\mu = \lambda\mu, \\ \mathcal{P}^\star\mu^\star = \lambda\mu^\star, \end{array}\right. \qquad \lambda = \sup \mathrm{Spectrum}(\mathcal{P}) = \sup \mathrm{Spectrum}(\mathcal{P}^\star). \tag{2.15}$$

Remark 5 *The operators $\mathcal{P}$ and $\mathcal{P}^\star$ depend on N, since they act on functions of $2N$ variables. Hence, the highest eigenvalue λ as well as the associated eigenvectors μ and $\mu^\star$ depend on N. To simplify the notation, we have not made this dependence explicit in* (2.15).

Assuming that the highest eigenvalue of $\mathcal{P}$ is simple and isolated, the equation (2.12) yields

$$\begin{aligned} x^\star &= \lim_{N\to+\infty} \frac{\displaystyle\int_{\mathbb{R}^N\times\mathbb{R}^N} x_{k,l}\ \mu(x_{:,l}, y_{:,l})\ \mu^\star(x_{:,l}, y_{:,l})\ dx_{:,l}\ dy_{:,l}}{\displaystyle\int_{\mathbb{R}^N\times\mathbb{R}^N} \mu(x_{:,l}, y_{:,l})\ \mu^\star(x_{:,l}, y_{:,l})\ dx_{:,l}\ dy_{:,l}} \\ &= \lim_{N\to+\infty} \frac{\displaystyle\int_{\mathbb{R}^N\times\mathbb{R}^N} x_k\ \mu(x,y)\ \mu^\star(x,y)\ dx\ dy}{\displaystyle\int_{\mathbb{R}^N\times\mathbb{R}^N} \mu(x,y)\ \mu^\star(x,y)\ dx\ dy}. \end{aligned} \tag{2.16}$$

In the above integrals, x denotes the vector $(x_1, \ldots, x_N) \in \mathbb{R}^N$, and $1 \ll k \ll N$.

Remark 6 *Note that approximating* (2.12)-(2.13) *by* (2.16) *consists in passing to the limit $N \to \infty$ faster in the vertical direction than in the horizontal direction. Indeed, the operator $\mathcal{P}$ acts on functions of $2N$ variables, which correspond to increments $\{x_{i,j}, y_{i,j}\}_{i=1,N}$, for some j. These are all the increments along a row of atoms in the horizontal direction. We hence freeze the number of particles in the horizontal direction and pass to the limit in the vertical direction, since we consider the eigenmode of highest eigenvalue of $\mathcal{P}$ and $\mathcal{P}^\star$.*

In order to take benefit from (and proceed further than) (2.16), we need to solve the eigenvalue problem (2.15). This problem is posed on functions on $2N$ variables. Solving this problem directly is hence out of reach numerically. The approach we suggest consists in further approximating the problem, arguing somewhat similarly to a mean-field theory. Using a sequence of simplifying assumptions (see in particular (2.19) below), we are going to derive an integrated form of (2.15) (see (2.20) and (2.21) below). Eventually, this will allow us to recover a Markov structure on *low* dimensional objects. The invariant measure of such Markov chain will hence be the solution of an eigenvalue problem, similarly to (2.15), but, in contrast to (2.15), in a low-dimensional setting, and thus amenable to numerical computations.

Before proceeding along these lines, we make the following observation. We note that any μ satisfying (2.15) is of the form

$$\begin{aligned}\forall (x,y) \in \mathbb{R}^N \times \mathbb{R}^N, \quad \mu(x,y) = F(x)F(y)\nu(x), \quad \text{with} \\ \forall x \in \mathbb{R}^N, \quad \lambda\, \nu(x) = \int_{\mathbb{R}^N} F(z)F(x+z-\tau z)\nu(x+z-\tau z)dz. \quad (2.17)\end{aligned}$$

Similarly, any $\mu^\star$ solution to (2.15) is of the form

$$\begin{aligned}\forall (x,y) \in \mathbb{R}^N \times \mathbb{R}^N, \quad \mu^\star(x,y) = F(x+\tau y - y)\ \nu^\star(x+\tau y - y), \quad \text{with} \\ \forall x \in \mathbb{R}^N, \quad \lambda\, \nu^\star(x) = \int_{\mathbb{R}^N} F(z)\ F(x+\tau z - z)\ \nu^\star(x+\tau z - z)\ dz. \quad (2.18)\end{aligned}$$

In the sequel, we describe a strategy to approximate ν and $\nu^\star$, which is based on a direct product ansatz. The functions ν and $\nu^\star$ depend on fewer variables than μ and $\mu^\star$, and are hence easier to handle.

2.2 A direct product ansatz

Considering that the problems (2.17) and (2.18) are (at least asymptotically) symmetric in the variables, we introduce the ansatz

$$\textbf{[H3]} \quad \nu(x) = \prod_{i=1}^N g(x_i), \quad \nu^\star(x) = \prod_{i=1}^N g^\star(x_i), \qquad (2.19)$$

insert it in (2.17) and (2.18), and integrate with respect to all x_i except one. This gives the following eigenproblems on g and $g^\star$:

$$\lambda g(x_i) = \int_{\mathbb{R}^2} f(x_i + z_i - z_{i-1}) f(z_i) f(z_{i-1}) g(x_i + z_i - z_{i-1}) dz_{i-1} dz_i, \quad (2.20)$$

$$\lambda g^\star(x_i) = \int_{\mathbb{R}^2} f(x_i + z_{i-1} - z_i) f(z_i) f(z_{i-1}) g^\star(x_i + z_{i-1} - z_i) dz_i dz_{i-1}, \quad (2.21)$$

where λ is the largest possible eigenvalue. Note that (2.20) and (2.21) are the same equation. Using the Krein-Rutman theorem [32], it is possible to prove that for many types of interactions, the corresponding eigenvalue is simple. Hence, $g = g^\star$. In addition, observe that (2.20) is an eigenvalue problem on functions of one variable: it can be solved numerically.

Using (2.17), (2.18) and (2.19), we thus have, up to a normalization factor, that, for any $(x, y) \in \mathbb{R}^{2N}$,

$$\mu(x,y) = \prod_{j=1}^{N} f(x_j) f(y_j) g(x_j), \quad \mu^\star(x,y) = \prod_{j=1}^{N} f(x_j + y_{j+1} - y_j) g(x_j + y_{j+1} - y_j), \quad (2.22)$$

where g is the solution of (2.20).

Remark 7 *Note that the direct product ansatz* (2.19) *does not imply that, in the law* (2.14) *of* $(x_{:,l}, y_{:,l})$*, the increments* $(x_{j,l}, y_{j,l})$*,* $j = 1, \dots, N$*, are independent. Indeed, in view of* (2.22)*, the numerator of* (2.14) *reads*

$$\mu(x_{:,l}, y_{:,l})\ \mu^\star(x_{:,l}, y_{:,l}) = \prod_{j=1}^{N} f(x_{j,l}) f(y_{j,l}) g(x_{j,l}) f(x_{j,l} + y_{j+1,l} - y_{j,l}) g(x_{j,l} + y_{j+1,l} - y_{j,l}),$$

which is not *a direct product of functions depending on* $(x_{j,l}, y_{j,l})_{j=1}^N$*.*

We now insert (2.22) in (2.16) and obtain

$$x^\star = \lim_{N \to +\infty} Z_N^{-1} \int_{\mathbb{R}^N \times \mathbb{R}^N} x_k \prod_{j=1}^{N} f(x_j) f(y_j) g(x_j) \times f(x_j + y_{j+1} - y_j) g(x_j + y_{j+1} - y_j)\ dxdy, \quad (2.23)$$

where $Z_N = \int_{\mathbb{R}^N \times \mathbb{R}^N} \prod_{j=1}^{N} f(x_j) f(y_j) g(x_j) f(x_j + y_{j+1} - y_j) g(x_j + y_{j+1} - y_j)\ dxdy$.

The Markov structure present in the right hand side of (2.23) now allows us to proceed. We introduce the transfer operator $\mathcal{Q}$ defined by

$$(\mathcal{Q}\psi)(x_{j+1}, y_{j+1}) = f(x_{j+1})\ f(y_{j+1}) \int_{\mathbb{R}^2} g(x_j) \times f(x_j + y_{j+1} - y_j)\ g(x_j + y_{j+1} - y_j)\ \psi(x_j, y_j)\ dx_j\ dy_j, \quad (2.24)$$

its adjoint $\mathcal{Q}^\star$, and the invariant measure equations

$$\left\{ \begin{array}{l} \mathcal{Q}\psi = \eta\psi, \\ \mathcal{Q}^\star\psi^\star = \eta\psi^\star, \end{array} \right. \qquad \eta = \sup \mathrm{Spectrum}(\mathcal{Q}) = \sup \mathrm{Spectrum}(\mathcal{Q}^\star). \tag{2.25}$$

Using $\mathcal{Q}$ and $\mathcal{Q}^\star$, we recast (2.23) as

$$x^\star = \lim_{N\to+\infty} \frac{\displaystyle\int_{\mathbb{R}^2} x_k \ \left(\mathcal{Q}^{k-1}\psi_0\right)(x_k,y_k) \ \left((\mathcal{Q}^\star)^{N-k}\psi_1\right)(x_k,y_k)\ dx_k\,dy_k}{\displaystyle\int_{\mathbb{R}^2} \left(\mathcal{Q}^{k-1}\psi_0\right)(x_k,y_k) \ \left((\mathcal{Q}^\star)^{N-k}\psi_1\right)(x_k,y_k)\ dx_k\,dy_k} \tag{2.26}$$

for some ψ_0 and ψ_1. Using again the Krein-Rutman theorem, we obtain that the highest eigenvalue of $\mathcal{Q}$ is simple and isolated, hence the iterations of $\mathcal{Q}$ converge, up to renormalization, to the projection on ψ, the eigenvector associated to the highest eigenvalue. We hence infer from (2.26) that

$$\begin{array}{rcl} x^\star & = & \displaystyle\frac{\displaystyle\int_{\mathbb{R}^2} x_k\,\psi(x_k,y_k)\,\psi^\star(x_k,y_k)\,dx_k\,dy_k}{\displaystyle\int_{\mathbb{R}^2} \psi(x_k,y_k)\,\psi^\star(x_k,y_k)\,dx_k\,dy_k}, \\ y^\star & = & \displaystyle\frac{\displaystyle\int_{\mathbb{R}^2} y_k\,\psi(x_k,y_k)\,\psi^\star(x_k,y_k)\,dx_k\,dy_k}{\displaystyle\int_{\mathbb{R}^2} \psi(x_k,y_k)\,\psi^\star(x_k,y_k)\,dx_k\,dy_k}. \end{array} \tag{2.27}$$

Note that, owing to the specific structure of $\mathcal{Q}$, its eigenvector $\psi(x,y)$ reads

$$\forall (x,y)\in\mathbb{R}\times\mathbb{R}, \quad \psi(x,y) = f(x)\,f(y)\,\overline{\psi}(y), \tag{2.28}$$

where, for any $y'\in\mathbb{R}$,

$$\eta\overline{\psi}(y') = \int_{\mathbb{R}^2} g(x)\,f(x+y'-y)\,g(x+y'-y)\,f(x)\,f(y)\,\overline{\psi}(y)\ dx\ dy. \tag{2.29}$$

Hence, computing the function ψ, which depends on *two* scalar variables, amounts to determining $\overline{\psi}$, namely solving an eigenvalue problem on functions of *one* variable. In a similar way, the eigenvector $\psi^\star(x,y)$ of $\mathcal{Q}^\star$ reads

$$\forall (x,y)\in\mathbb{R}\times\mathbb{R}, \quad \psi^\star(x,y) = g(x)\,\overline{\psi}^\star(x-y), \tag{2.30}$$

with, for any $x\in\mathbb{R}$,

$$\eta\overline{\psi}^\star(x) = \int_{\mathbb{R}^2} f(x'+y')\,f(y')\,f(x+y')\,g(x+y')\,g(x'+y')\,\overline{\psi}^\star(x')\ dx'\ dy'. \tag{2.31}$$

Again, we are left with solving an eigenvalue problem on a function of *one* variable.

2.3 Summary

The above approach results in an algorithm for computing an approximation of $\langle A \rangle_N$. This algorithm may be summarized as follows:

1. compute the function $g : \mathbb{R} \mapsto \mathbb{R}$ satisfying the eigenvalue equation (2.20). Note that λ should be the largest eigenvalue of the corresponding operator;

2. with g, compute the operator $\mathcal{Q}$ given by (2.24), and compute the functions ψ and $\psi^\star$ solution to (2.25); this amounts in practice to solving the eigenvalue problems (2.29) and (2.31) for $\overline{\psi} : \mathbb{R} \mapsto \mathbb{R}$ and $\overline{\psi}^\star : \mathbb{R} \mapsto \mathbb{R}$, where again η is the largest eigenvalue; the functions ψ and $\psi^\star$ are next computed using (2.28) and (2.30);

3. with ψ and $\psi^\star$, compute $x^\star$ and $y^\star$ given by (2.27);

4. approximate the limit of $\langle A \rangle_N$ by $A(x^\star + y^\star)$, following (2.9).

Remark 8 *As pointed out in Remark 4, our strategy can also handle observables that depend on $u^{N,N}$, $u^{N,0}$ and $u^{0,N}$. We then take the approximation*

$$\lim_{N \to \infty} \langle A\left(u^{N,N}, u^{N,0}, u^{0,N}\right) \rangle_N \approx A(x^\star + y^\star, x^\star, y^\star).$$

2.4 The Gaussian case

In this section, we consider the special case when, in (1.16), we choose

$$W(x) = x^2, \quad f(x) = \exp(-\beta W(x)) = \exp(-\beta x^2).$$

Let us show that, in this case, our strategy formally yields the correct value for $x^\star$ and $y^\star$. To simplify the notation, we assume henceforth that the inverse temperature is $\beta = 1$.

First, since μ_N is an even function, we infer from (2.7) that $x^\star = 0$. Let us now follow our strategy, as summarized in Section 2.3 above. Taking the Fourier transform of the equation (2.20), we have

$$\lambda \widehat{g}(\omega) = \widehat{f}(\omega)\widehat{f}(-\omega)\widehat{fg}(\omega).$$

This is an eigenvalue problem, and we are interested in the case when λ is maximal. In such a case, and under mild assumptions on f (see [6] for the details), one easily proves that the corresponding solution g is unique and never vanishes. In addition, any other eigenvector must vanish at some point of $\mathbb{R}$ (see [14, Chap. 1, Theorem 1.2]). Hence, if we find a non-vanishing solution of the above problem, it is the unique solution we are looking for. Postulating that $g(x) = \exp(-\alpha x^2)$ for some α, we deduce from the above relation that α should satisfy $1 = 2\alpha + 2\alpha^2$. This equation has two real solutions, and only one of them is positive. It thus determines $\alpha > 0$. This gives us a positive solution, which, according to the above argument, corresponds to the largest possible λ.

We now consider the eigenvalue problem (2.29). Taking the Fourier transform of this equation, and postulating that $\overline{\psi}(x) = \exp(-\tau x^2)$ for some τ, we find that τ should satisfy $1 + \alpha = 2\tau + 2\tau^2$. Again, this equation has two real solutions, and only one of them is positive. It thus determines $\tau > 0$.

We finally turn to the eigenvalue problem (2.31), and assume that its solution reads $\overline{\psi}^\star(x) = \exp(-\gamma x^2)$ for some γ. A tedious computation then shows that γ should satisfy

$$\frac{1}{\gamma} = \frac{1}{1+\alpha} + \frac{1}{1+\tau} > 0.$$

Having identified the functions g, $\overline{\psi}$ and $\overline{\psi}^\star$, we can now evaluate the right-hand side of (2.27). Since f, g, $\overline{\psi}$ and $\overline{\psi}^\star$ are even functions, we note that

$$\psi(x,y)\psi^\star(x,y) = f(x)f(y)\overline{\psi}(y)\ g(x)\overline{\psi}^\star(x-y) = \psi(-x,-y)\psi^\star(-x,-y).$$

Using the change of variable $(x,y) \mapsto (-x,-y)$ in the right-hand side of (2.27), we deduce that

$$\frac{\displaystyle\int_{\mathbb{R}^2} x\,\psi(x,y)\,\psi^\star(x,y)\,dx\,dy}{\displaystyle\int_{\mathbb{R}^2} \psi(x,y)\,\psi^\star(x,y)\,dx\,dy} = 0.$$

Consequently, our strategy yields the exact result, namely $x^\star = 0$. In the following section, we numerically consider a more generic case, for which no analytical solution is available.

3 Numerical results

For our numerical simulations, we choose the interaction potential

$$W(x) = \frac{1}{2}(x-1)^4 + \frac{1}{2}x^2.$$

Note that W is not an even function, neither does it satisfy $\displaystyle\int_{\mathbb{R}} x\exp(-\beta W(x))\,dx = 0$. Hence the difference in height over a given edge of the membrane lattice does not average to 0. For a given choice of the inverse temperature β, we have followed the strategy summarized in Section 2.3, that yields $x^\star$ and $y^\star$ defined by (2.27). This allows to compute the reduced model results, that is, the quantity $A(x^\star + y^\star)$, for any given observable A.

The reference model result is $\langle A\rangle_N$ defined by (1.17). To compute this quantity, we resort to the stochastic differential equation

$$du_t = -\nabla_u E(u_t)\,dt + \sqrt{2\beta^{-1}}\,dB_t \quad \text{in } \mathbb{R}^{(N+1)^2-1}, \tag{3.1}$$

where B_t is a standard Brownian motion in dimension $(N+1)^2 - 1$. Of course, this is a very expensive way of computing $\langle A\rangle_N$, and we use it only to validate our approach, which is far less computationally demanding (see Table 1 below,

where we compare computational costs). As recalled in the Introduction, under mild assumptions on the potential W and the observable A, that are here satisfied, an ergodic theorem holds, and the canonical average (1.17) is given by

$$\langle A \rangle_N = \lim_{T \to \infty} \frac{1}{T} \int_0^T A\left(u_t^{N,N}\right) \, dt,$$

for (almost) all initial conditions $u_{t=0}$. In practice, the equation (3.1) is numerically integrated with the forward Euler scheme (also called the Euler-Maruyama scheme)

$$u_{m+1} = u_m - \Delta t \, \nabla_u E(u_m) + \sqrt{2\Delta t \beta^{-1}} \, G_m \tag{3.2}$$

where G_m is a vector of Gaussian random variables in dimension $(N+1)^2 - 1$, and Δt is a small time step. In turn, the canonical average is approximated by

$$\langle A \rangle_N \approx \lim_{M \to \infty} \frac{1}{M} \sum_{m=1}^{M} A\left(u_m^{N,N}\right). \tag{3.3}$$

In practice, we have integrated (3.1) (using the scheme (3.2)) for a large but finite number M of time steps. We thus take the approximation

$$\langle A \rangle_N \approx \frac{1}{M} \sum_{m=1}^{M} A\left(u_m^{N,N}\right) \tag{3.4}$$

for large M and small Δt. The deterministic quantity $\langle A \rangle_N$ is thus approximated by a random number. To compute error bars for $\langle A \rangle_N$ (that is, confidence intervals), we have simulated many independent realizations of the dynamics (3.1).

The reference model results reported here have been obtained using (3.2)-(3.3) with $\Delta t = 10^{-3}$ and a number of time steps M large enough such that convergence is reached in (3.3), up to statistical noise.

3.1 Average of observables: convergence with N

In Figures 2 and 3, we compare the reference observable average $\langle A \rangle_N$ with its approximation $A(x^\star + y^\star)$, for several observables A, and for increasing values of N (the temperature is fixed at $\beta^{-1} = 1$). We observe a good agreement between $A(x^\star + y^\star)$ and $\langle A \rangle_N$, the latter seeming indeed to converge to the former, when $N \to \infty$: for $N = 100$, the relative difference is of about 1%.

In Figure 4, we compare $\langle u^{N,0} \rangle_N$ with $x^\star$, in line with Remark 8. We again observe a good agreement between the reduced model and the reference model results. On the same figure, we compare $\langle u^{0,N} \rangle_N$ with $y^\star$, with similar conclusions.

For the sake of completeness, we compare in Table 1 the costs for computing the reference value $\langle A \rangle_N$ with those associated to the reduced model approach. We clearly see that the latter are much smaller than the former.

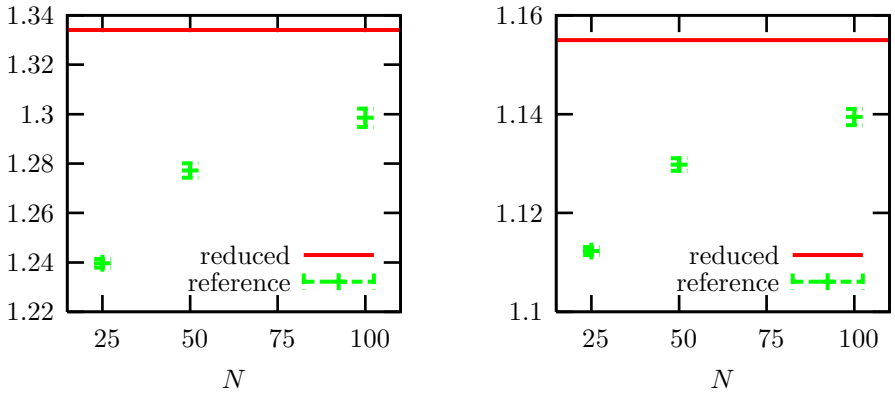

Figure 2: Comparison of $\langle A \rangle_N$ (reference result, defined by (1.17)), with $A(x^\star + y^\star)$ (reduced model result), for several values of N ($\beta = 1$; left: $A(u) = u^2$; right: $A(u) = u$).

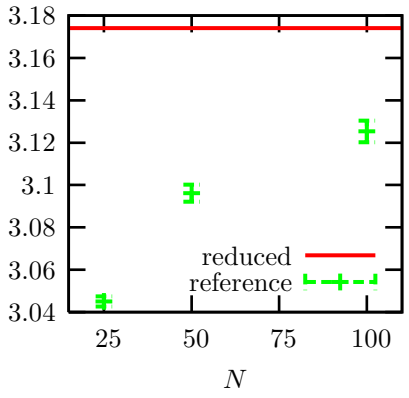

Figure 3: Comparison of $\langle A \rangle_N$ (reference result defined by (1.17)), with $A(x^\star + y^\star)$ (reduced model result), for several values of N ($A(u) = \exp(u)$, $\beta = 1$).

	$N = 25$	$N = 50$	$N = 100$	Reduced model
CPU time (days)	0.2	0.7	4.6	0.025

Table 1: First 3 columns: CPU time for computing the reference value $\langle A \rangle_N$ (for *one* choice of observable A, at *one* given temperature) using the approximation (3.4) along *one* single realization of (3.2), with $\Delta t = 10^{-3}$ and $M = 10^8$ time steps. Last column: CPU time needed by the algorithm of Section 2.3 (in practice, eigenproblems have been solved on the interval $I = [-4; 5]$, using a spectral basis of 20 functions; integrals on the interval I have been computed using the 6 Gauss points quadrature rule, discretizing I into 20 subintervals).

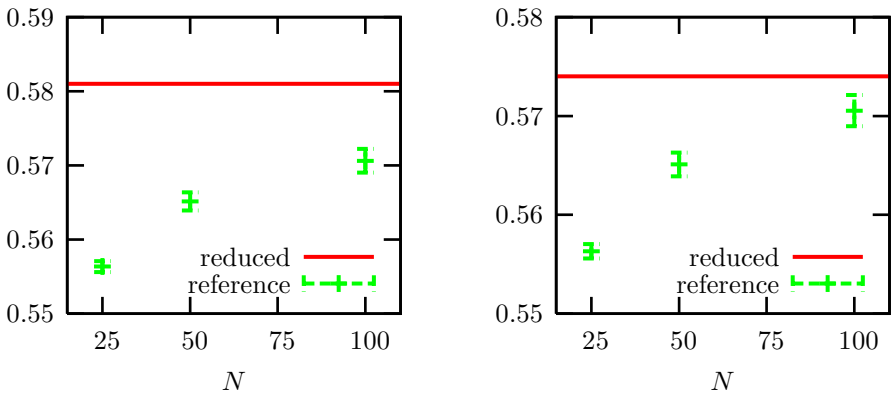

Figure 4: Left: Comparison of $\langle u^{N,0}\rangle_N$ (reference result) with $x^\star$ (reduced model result), for several values of N ($\beta = 1$). Right: Comparison of $\langle u^{0,N}\rangle_N$ (reference result) with $y^\star$ (reduced model result).

3.2 Average of observables: temperature dependence

In Figures 5 and 6, we compare the reference observable average $\langle A\rangle_N$ with its approximation $A(x^\star + y^\star)$, for several observables A, and for different temperatures (the reference system is run with $N = 100$ particles in each direction). We observe a good agreement between $A(x^\star+y^\star)$ and $\langle A\rangle_N$, for all the temperatures considered.

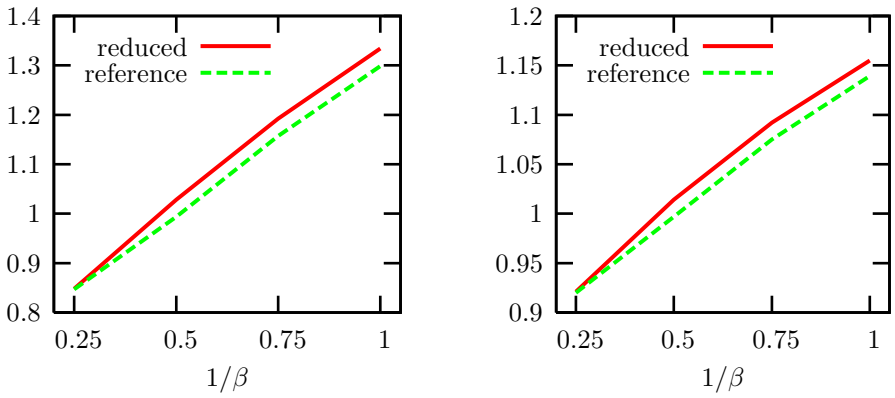

Figure 5: Comparison of $\langle A\rangle_N$ (reference result defined by (1.17)), with $A(x^\star + y^\star)$ (reduced model result), as a function of the inverse temperature β ($N = 100$; left: $A(u) = u^2$; right: $A(u) = u$).

On Figure 7, we compare $\langle u^{N,0}\rangle_N$ (respectively $\langle u^{0,N}\rangle_N$) with $x^\star$ (respectively $y^\star$). We again observe a good agreement between the reduced model and

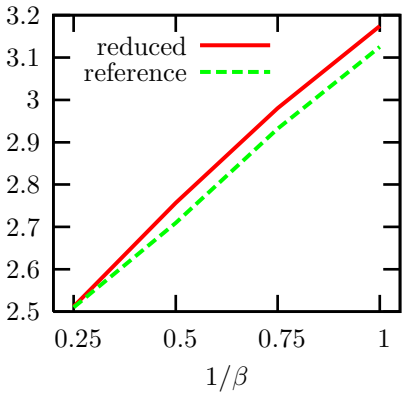

Figure 6: Comparison of $\langle A \rangle_N$ (reference result defined by (1.17)), with $A(x^\star + y^\star)$ (reduced model result), as a function of the inverse temperature β ($A(u) = \exp(u)$, $N = 100$).

the reference model results, for all the temperatures we have tested.

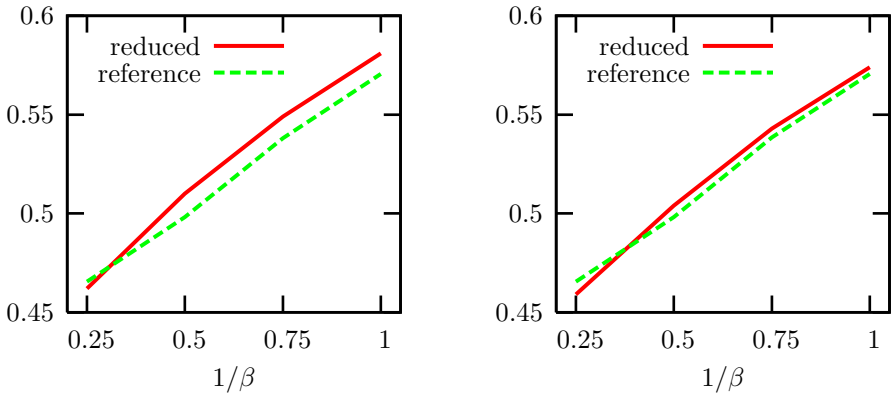

Figure 7: Left: Comparison of $\langle u^{N,0} \rangle_N$ (reference result) with $x^\star$ (reduced model result), as a function of the inverse temperature β ($N = 100$). Right: Comparison of $\langle u^{0,N} \rangle_N$ (reference result) with $y^\star$ (reduced model result).

3.3 Correlations

In this section, we compare the correlations of successive increments in the membrane. More precisely, we compute, according to the reference model and the reduced model, the average of products of the type $x_{k,l} x_{k+p,l}$ for some $p \geq 0$.

Recall that

$$x_{k,l} = \frac{u^{k,l} - u^{k-1,l}}{h}$$

is the (rescaled) difference in height between atoms at sites $(k-1,l)$ and (k,l). This kind of tests are more demanding than the ones considered above.

The reference model computations have been performed on a system of $(N+1)^2$ atoms. The correlation can be defined from all the increments except those at the boundaries, or just the increments at the center of the system. Both yield very close results (the difference is smaller than 0.2 %). In addition, those reference computations have been computed by averaging several independent realizations. The number of realizations we have considered is large enough so that the statistical noise is smaller (in relative error) than 0.2 %. Results given by the reference computations are gathered in the second column of Table 2.

The reduced model values have been computed by starting from the exact values, e.g.

$$\langle x_{k,l}^2 \rangle = Z_N^{-1} \int x_{k,l}^2 \; \mu_N \left(\{x_{i,j}\}, \{y_{i,j}\} \right),$$

and following the steps described in Section 2. This yields the quantity

$$\langle x_{k,l}^2 \rangle_{\rm red} = \frac{\displaystyle\int_{\mathbb{R}^2} x_k^2 \, \psi(x_k, y_k) \, \psi^\star(x_k, y_k) \, dx_k \, dy_k}{\displaystyle\int_{\mathbb{R}^2} \psi(x_k, y_k) \, \psi^\star(x_k, y_k) \, dx_k \, dy_k} \tag{3.5}$$

as an approximation of $\langle x_{k,l}^2 \rangle$. In turn, the quantity $\langle x_{k,l} \; x_{k+1,l} \rangle$ is approximated by

$$\langle x_{k,l} \; x_{k+1,l} \rangle_{\rm red} = \frac{\displaystyle\int_{\mathbb{R}^4} x_k x_{k+1} \, \psi(x_k, y_k) \, c(x_k, y_k, x_{k+1}, y_{k+1}) \, \psi^\star(x_{k+1}, y_{k+1}) \, dx_k \, dy_k \, dx_{k+1} \, dy_{k+1}}{\displaystyle\int_{\mathbb{R}^4} \psi(x_k, y_k) \, c(x_k, y_k, x_{k+1}, y_{k+1}) \, \psi^\star(x_{k+1}, y_{k+1}) \, dx_k \, dy_k \, dx_{k+1} \, dy_{k+1}}, \tag{3.6}$$

with

$$c(x_k, y_k, x_{k+1}, y_{k+1}) = g(x_k) \, f(x_{k+1}) \, f(y_{k+1}) \, g(x_k + y_{k+1} - y_k) \, f(x_k + y_{k+1} - y_k).$$

Note that formulas (3.5) and (3.6) are consistent with each other. Indeed, if

$x_{k+1,l}$ is replaced by $x_{k,l}$ in (3.6), we have

$$\begin{aligned}
&\langle x_{k,l}\ x_{k,l}\rangle_{\mathrm{red}} \\
= &\frac{\displaystyle\int_{\mathbb{R}^4} x_k^2\,\psi(x_k,y_k)\,c(x_k,y_k,x_{k+1},y_{k+1})\,\psi^\star(x_{k+1},y_{k+1})\,dx_k\,dy_k\,dx_{k+1}\,dy_{k+1}}{\displaystyle\int_{\mathbb{R}^4} \psi(x_k,y_k)\,c(x_k,y_k,x_{k+1},y_{k+1})\,\psi^\star(x_{k+1},y_{k+1})\,dx_k\,dy_k\,dx_{k+1}\,dy_{k+1}} \\
= &\frac{\displaystyle\int_{\mathbb{R}^2} x_k^2\,\psi(x_k,y_k)\,(\mathcal{Q}^\star\psi^\star)(x_k,y_k)\,dx_k\,dy_k}{\displaystyle\int_{\mathbb{R}^2} \psi(x_k,y_k)\,(\mathcal{Q}^\star\psi^\star)(x_k,y_k)\,dx_k\,dy_k} \\
= &\frac{\displaystyle\int_{\mathbb{R}^2} x_k^2\,\psi(x_k,y_k)\,\psi^\star(x_k,y_k)\,dx_k\,dy_k}{\displaystyle\int_{\mathbb{R}^2} \psi(x_k,y_k)\,\psi^\star(x_k,y_k)\,dx_k\,dy_k}
\end{aligned}$$

and we recover (3.5). We have used in the above derivation the fact that

$$\int_{\mathbb{R}^2} c(x_k,y_k,x_{k+1},y_{k+1})\,\psi^\star(x_{k+1},y_{k+1})\,dx_{k+1}\,dy_{k+1} = \mathcal{Q}^\star\psi^\star(x_k,y_k) = \eta\psi^\star(x_k,y_k).$$

Integrals in dimension 2 and 4 need to be evaluated to compute (3.6) (and similarly, integrals in dimension 6 need to be evaluated to compute $\langle x_{k,l}\ x_{k+2,l}\rangle_{\mathrm{red}}$). These integrals have been computed almost exactly using numerical quadratures. We gather the obtained results in the third column of Table 2.

	Reference model	Reduced model	Relative difference
$\langle x_{k,l}^2\rangle$	0.50668	0.52808	4.05×10^{-2}
$\langle y_{k,l}^2\rangle$	0.50684	0.51217	1.04×10^{-2}
$\langle x_{k,l}\ x_{k+1,l}\rangle$	0.28097	0.31697	0.114
$\langle x_{k,l}\ x_{k+2,l}\rangle$	0.31215	0.33089	5.66×10^{-2}
$\langle x_{k,l}\rangle$	0.57310	0.581	1.36×10^{-2}

Table 2: Comparison of the correlations of successive increments according to the reduced model with the reference model values (inverse temperature $\beta = 1$, $N = 100$, $1 \ll k, l \ll N$). The reference values are expectations (e.g. of $x_{k,l}^2$) with respect to the Gibbs measure $Z_N^{-1}\overline{\mu}_N$ defined by (1.18).

We observe that the difference between the reference result and the reduced model results is of the order of 5% for all values except one. We consider that such an accuracy is good, given the number of assumptions on which the numerical strategy leading to the reduced model values is based.

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